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Light-matter interaction between photonic bound states in the continuum and bright excitons in transition metal dichalcogenides

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Abstract. Being motivated by recent achievements in the rapidly developing fields of optical bound states in the continuum (BICs) and excitons in monolayers of transition metal dichalcogenides, we analyze strong coupling between BICs in Ta₂O₅ periodic photonic structures and excitons in WSe₂ monolayers. We demonstrate that giant radiative lifetime of BICs allow to engineer the exciton-polariton lifetime enhancing it three orders of magnitude compared to a bare exciton.

1. Introduction

Monolayers of transition metal dichalcogenides (TMDCs) are a certain class of post-graphene two-dimensional materials [1], attracting vast research interest in recent years. TMDC are direct-gap semiconductors, exhibiting strong light-matter coupling [2], leading to the emergence of the new quasiparticles, exciton-polaritons [3] at room temperatures in structures comprising TMDC monolayer and an optical cavity.

Excitons-polaritons have been extensively studied in last two decades due to their fascinating fundamental properties. Strong coupling of TMDC excitons to light has been observed in the structures resembling the conventional microcavities, where the monolayer was sandwiched between two Bragg mirrors [4]. At the same time, since fabrication of high quality TMDC monolayers is based on the mechanical exfoliation techniques, it is quite technologically demanding. Thus, it would be extremely useful to realize high quality optical resonances without the requirement for the growth of the upper mirror.

In this paper we propose an alternative scheme for the realization of strong exciton-photon coupling in 2D materials without using mirrors which is beneficial both in terms of ease of realization and tunability. We focus on structures comprising of a TMDC and a photonic crystal slab (PCS). The idea behind that is the exploitation of the so-called optical bound state in the continuum (BIC) [5], supported by the PCS, as a high quality cavity mode. BICs in the periodic photonic structures originate due to destructive interference of the leaky modes supported by the PCS. They are characterized by extremely high quality factors.

The design of structure is shown in Fig. 1 - a WSe₂ flake is placed on top of an one-dimensional Ta₂O₅ PCS. We notice that strong light-matter coupling demands both high-Q



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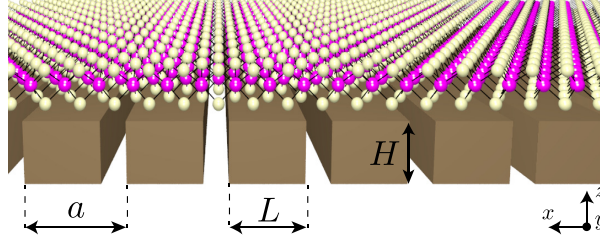


Figure 1. Isometric view of a PCS-TMDC structure. The refractive index of Ta_2O_5 bars is equal to 2.1. The TMDC made of WSe_2 is laid on top of the PhC slab.

photonic structures and long-living excitonic states. We address this problem by tuning the PCS shape and material parameters to the regime of bound states in the continuum providing a giant quality factor of resonator which is limited by surface roughness and finite size of the sample only.

We begin with analysis of the eigenmode spectrum of the PCS applying the guided-mode expansion (GME) method [6] widely used for characterization of photonic eigenmodes of periodic photonic structures.

We consider an air-suspended Ta_2O_5 one-dimensional grating with lower and upper air claddings being semi-infinite. The PCS consists of rectangular bars with height H and width L being spaced equidistant with a period of a (see Fig. 1). We put refractive index of Ta_2O_5 equal to 2.1 which is appropriate for the red band of the visible spectrum range. The calculations are performed for the PCS with $a = 1.03H$, $L = 0.90a$ and the eigenvalue problem is truncated by 101 plane waves and 8 guided modes of the effective waveguide kept in the expansion [6]. The spectrum of eigenfrequencies ω and inverse radiation lifetimes $\gamma = 1/(2\tau_{\text{rad}})$ of the PCS for in-plane wavevectors along the x direction of the first Brillouin zone is shown in Fig. 2(a,c) for TE-polarized and in Fig. 2(b,d) for TM-polarized modes, respectively. The BICs represent unusual leaky modes with $\gamma = 0$ and can be formed both at the center of the Brillouin zone (at- Γ BIC) and at specific points between the zone edge and center (off- Γ BIC).

Optical properties of WSe_2 monolayers are governed by very robust excitons with binding energies of the order of 500 meV [7]. We study A-type excitons representing bound states of electrons in the conduction band and holes in the upper subband of the valence band of \mathbf{K}_+ and \mathbf{K}_- valleys [8]. We focus on bright excitonic states active for in-plane polarization of incident light, which represent, in general, a pair of valley-degenerate states with σ_{\pm} polarization. In this case a linearly polarized pump excites a superposition of excitons with total polarization along the in-plane component of the electric field of light.

To investigate light-matter interaction between excitons in the TMDC monolayer and BICs in the PCS we apply the full quantum formalism for both photonic and excitonic states being an extension of the GME method [9]. Coupling between photonic and exciton modes is governed by the oscillator strength f and the overlap integral of mode profiles

$$V_{n,\mathbf{k}_{\parallel}} = -i\sqrt{f} \int_{\text{cell}} d\mathbf{r}_{\parallel} \mathbf{e} \cdot \mathbf{E}_{n,\mathbf{k}_{\parallel}}^{\text{up}}(\mathbf{r}_{\parallel}) e^{-i\mathbf{k}_{\text{exc}}\mathbf{r}_{\parallel}}. \quad (1)$$

Here \mathbf{e} is the unit vector of exciton polarization, \mathbf{k}_{\parallel} and \mathbf{k}_{exc} are in-plane wavevectors of light and exciton, respectively, and $\mathbf{E}_{n,\mathbf{k}_{\parallel}}^{\text{up}}$ is the electric field of n -th photonic mode at the upper surface of the PCS. Importantly, exciton-photon interaction is allowed only under condition $\mathbf{k}_{\text{exc}} = \mathbf{k}_{\parallel} + \mathbf{G}$, where \mathbf{G} is the reciprocal lattice vector. We formulate the total Hamiltonian and reduce it to a non-Hermitian eigenvalue equation.

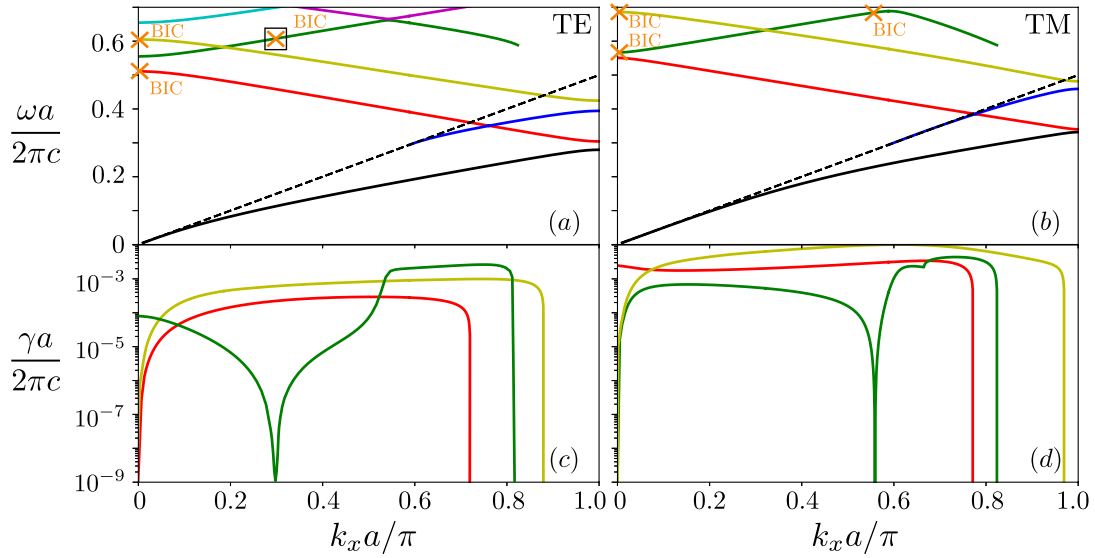


Figure 2. Eigenmode spectrum of air-suspended Ta_2O_5 one-dimensional grating. Band structure $\omega a/2\pi c$ for (a) TE-polarized and (b) TM-polarized modes, respectively. Black dashed lines represent the light lines $\omega = ck_x$. Dimensionless inverse radiation lifetime $\gamma a/2\pi c$ for (c) TE-polarized and (d) TM-polarized modes, respectively. BICs are marked by orange crosses.

We apply the procedure for characterization of band structure and damping rates of exciton-polaritons being formed in the vicinity of the BIC. At low temperatures of about 4 K energy of A-type bright exciton in WSe_2 is of order of $E_{\text{exc}} = 1.74$ eV [10] and its dispersion can be neglected at the scales of the problem. The radiative $\tau_{\text{exc,R}}$ and non-radiative $\tau_{\text{exc,NR}}$ lifetimes can be estimated as 1 ps [11] and 1 ns [12]. For a bare exciton, radiative channel dominates and leads to the damping rate $\hbar/(2\tau_{\text{exc}}) = 0.33$ meV. However, when the TMDC is strongly coupled to the PCS, the radiative channel of exciton into the photonic system is enabled and it dominates with respect to direct radiation into free space [13]. It leads to renormalization of exciton radiative lifetime of exciton used as a parameter for eigenmode procedure. Therefore, in calculations we use non-radiative lifetime for the exciton damping rate $\hbar/(2\tau_{\text{exc,NR}}) = 0.33 \mu\text{eV}$. Oscillator strength depends on $\tau_{\text{exc,R}}^{-1}$ and is about $6.5 \times 10^{-12} \text{ cm} \cdot \text{eV}^2$. We focus on the off- Γ BIC marked with a black square in Fig. 2 which has TE polarization which leads to better coupling with in-plane excitons according to Eq. 1. We tune the BIC frequency to a resonance with E_{exc} adjusting the height of the PCS to the value of $H = 418$ nm.

The spectrum of energies $\hbar\omega$ and inverse lifetimes $\hbar/(2\tau)$ of upper and lower exciton-polariton branches (UP and LP, respectively) calculated by means of the GME is shown in Fig. 3(a,b). Figure 3(a) demonstrates strong coupling between the exciton and the off- Γ BIC which manifests itself as an avoided resonance crossing with Rabi splitting of order of 3 meV. The radiation losses of both exciton-polariton branches are shown in Fig. 3(b) in comparison with the losses of photonic and exciton modes. As it can be seen, for specific values of k_x the lifetime of polariton modes can exceed the bare exciton lifetime by almost three orders of magnitude and reaches 0.66 ns. Such giant enhancement is the special effect intrinsic to optical bound states in the continuum. As it was discussed before, direct radiation of excitons into free space is strongly suppressed due to coupling to the PCS. At the same time BICs are entirely uncoupled to the radiation continuum. In total, this leads to suppression of all possible mechanisms of radiation resulting in giant LP lifetime comparable with the non-radiative lifetime of a bare exciton.

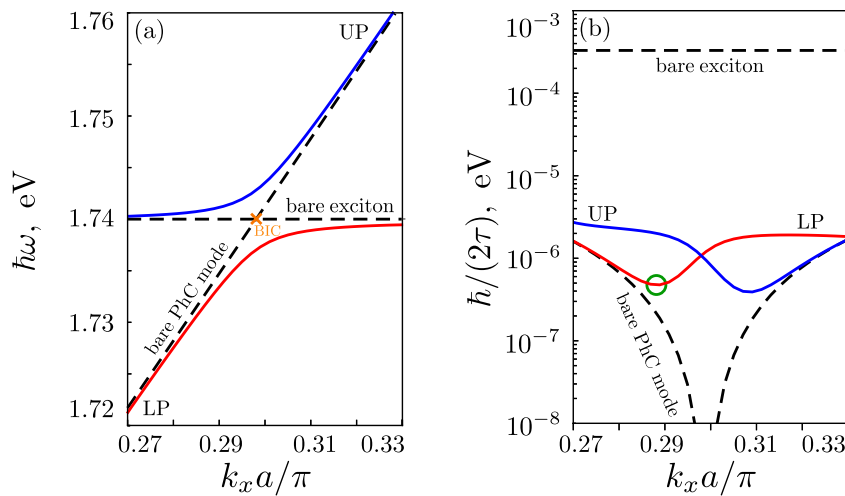


Figure 3. (a) Dispersion and (b) inverse lifetime of exciton-polaritons at the conditions of strong coupling between the TE-polarized photonic mode supporting an off- Γ BIC and in-plane polarized exciton with energy of 1.74 eV. State with maximal lifetime is marked by a green circle.

In conclusion, we have proposed an experimentally feasible scheme to achieve strong coupled exciton-photon system in a two-dimensional nanostructure comprising a TMDC monolayer and a periodic photonic nanostructure. Importantly, this scheme does not require the growth of Bragg mirrors, which substantially simplifies the fabrication. We believe, these findings open new avenues for the applications of strong light-matter coupling at the nanoscale.

Acknowledgments

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